N.S.G-225-63

UNPUBLISHED PRELIMINARY DATA

23p.

X63 15399

CODE-~~2f~~ 2d

THEORETICAL CHEMISTRY INSTITUTE

(2)

THE UNIVERSITY OF WISCONSIN

(1)

(NASA CR 51090)

A THREE-DIMENSIONAL ADDITION THEOREM FOR ARBITRARY

FUNCTIONS INVOLVING EXPANSIONS IN

SPHERICAL HARMONICS

by

R. A. Sack

WIS-TCI-24

25 July 1963

MADISON, WISCONSIN

Double code

A THREE-DIMENSIONAL ADDITION THEOREM FOR ARBITRARY FUNCTIONS INVOLVING EXPANSIONS IN SPHERICAL HARMONICS*

1884006

by

R. A. Sack (Chicago U. and

Department of Mathematics, Royal College of Advanced Technology)
Salford 5, England†

and

Theoretical Chemistry Institute, University of Wisconsin
Madison, Wisconsin

July 25, 1963 16 refs Submitted for Publication

ABSTRACT

15399

For any vector $\underset{\sim}{r} = \underset{\sim}{r}_1 + \underset{\sim}{r}_2$ an expansion is derived for the product of a power r^N of its magnitude and a surface spherical harmonic $Y_L^M(\vartheta, \varphi)$ of its polar angles in terms of spherical harmonics of the angles (ϑ_1, φ_1) and (ϑ_2, φ_2). The radial factors satisfy simple differential equations; their solutions can be expressed in terms of hypergeometric functions of the variable $(r_< / r_>)^2$, and the leading coefficients by means of Gaunt's coefficients or 3j-symbols. A number of linear transformations and three-term recurrence relations between the radial function are derived; but in contrast to the case $L = 0$ no generally valid expressions symmetric in r_1 and r_2 could be found.

By interpreting the terms operationally an expansion is derived for the product of $Y_L^M(\vartheta, \varphi)$ and an arbitrary function $f(r)$. The radial factors are expansions in derivatives of $f(r_>)$; for spherical waves they factorize into Bessel functions of r_1 and r_2 in agreement with the expansion by Friedman and Russek.

The 3j-symbols are briefly discussed in an un-normalized form; the new coefficients are integers, satisfying a simple recurrence relation through which they can be arranged on a 5-dimensional generalization of Pascal's triangle.

- - - - - -

* Supported in part by National Aeronautics and Space Administration (NASA Grant NsG-275-62 ~~(4180).~~ This work was begun at the Laboratory of Molecular Structure and Spectra, University of Chicago, supported by Office of Naval Research, Contract Nonr-2121(01))

† Permanent address.

A THREE-DIMENSIONAL ADDITION THEOREM FOR ARBITRARY FUNCTIONS INVOLVING EXPANSIONS IN SPHERICAL HARMONICS

1. Introduction

In a preceding paper[1] (referred to as I) a generalization was derived of Laplace's expansion for the inverse distance between two points Q_1 and Q_2, specified by the vectors r_1 and r_2 or the spherical polar coordinates $(r_1, \vartheta_1, \varphi_1)$ and $(r_2, \vartheta_2, \varphi_2)$. It was shown that in the expansion for an arbitrary power of the distance in terms of Legendre polynomicals of $(\cos \vartheta_{12})$

$$|r_2 - r_1|^n = \sum R_{n\ell}(r_1, r_2) P_\ell(\cos \vartheta_{12}) \qquad ; \tag{1}$$

the radial functions $R_{n\ell}$ can be expressed in terms of hypergeometric functions of the argument $(r_< / r_>)^2$, and by giving the expressions an operational interpretation an addition theorem was obtained valid for arbitrary analytic functions of $|r_2 - r_1|$.

A more general addition theorem would apply to functions $H(\underset{\sim}{r}_2 - \underset{\sim}{r}_1)$ or $H(\underset{\sim}{r}_2 + \underset{\sim}{r}_1)$ depending on the direction as well as on the magnitude of the vector argument. In Cartesian coordinates such an expansion is given by Taylor's theorem in three variables; in many physical applications, however, it is of advantage to specify the dependence on the angles in terms of spherical harmonics. These harmonics can be defined in several ways in terms of the associated Legendre functions $P_\ell^m(x)$

$$P_\ell^{|m|}(x) = (-)^m (1-x^2)^{\frac{1}{2}|m|} \frac{d^{|m|} P_\ell(x)}{dx^{|m|}} \quad ; \quad P_\ell^{-m}(x) = (-)^m P_\ell^m(x) \frac{(\ell - m)!}{(\ell + m)!} \; . \tag{2}$$

The most useful definitions are for the un-normalized harmonics

- - - - - -

[1] R. A. Sack, University of Wisconsin, Report WIS-TCI-20.

$$\Theta_\ell^m(\vartheta,\varphi) = e^{im\varphi} P_\ell^{|m|}(\cos\vartheta) \quad , \quad \Omega_\ell^m(\vartheta,\varphi) = e^{im\varphi} P_\ell^m(\cos\vartheta) \tag{3a,b}$$

and the normalized form

$$Y_\ell^m(\vartheta,\varphi) = \left[(2\ell+1)(\ell-m)!/4\pi(\ell+m)!\right]^{\frac{1}{2}} e^{im\varphi} P_\ell^m(\cos\vartheta) \quad . \tag{3c}$$

The functions $P_\ell(\cos\vartheta_{12})$ in (1) can be written as

$$P_\ell(\cos\vartheta_{12}) = \sum_{m=-\ell}^{\ell} (-)^m \, \Omega_\ell^{-m}(\vartheta_1,\varphi_1) \, \Omega_\ell^m(\vartheta_2,\varphi_2) \quad , \tag{4}$$

with corresponding expressions in terms of Θ or Y (cf. B 3.11.2)[2]. The purpose of the present paper is to derive the expansion for the product of a spherical harmonic and a power of the radius

$$V_{NML} = r^N \Omega_L^M(\vartheta,\varphi) = \sum R(N;L,\ell_1,\ell_2,M,m_1,m_2;r_1,r_2) \, \Omega_{\ell_1}^{m_1}(\vartheta_1,\varphi_1) \, \Omega_{\ell_2}^{m_2}(\vartheta_2,\varphi_2) \tag{5}$$

and its generalization for functions of the type $f(r)\Omega_L^M(\vartheta,\varphi)$. In contrast to I, the vector $\underset{\sim}{r} = (r,\vartheta,\varphi)$ denotes the sum of $\underset{\sim}{r}_1$ and $\underset{\sim}{r}_2$; the corresponding expressions for the difference $(\underset{\sim}{r}_2 - \underset{\sim}{r}_1)$ differ from those in (5) at most by a sign, corresponding to the parity of ℓ_1. The spherical harmonics in (5) could equally well be expressed in terms of Θ or Y ; the corresponding radial functions R_Θ and R_Y differ from $R \equiv R_\Omega$ only by a factor which is easily calculated from (2) and (3). In view of the transformation properties of the normalized functions Y their use would have the advantage that the azimuthal quantum numbers $m = M$, m_1, m_2 can affect the expressions

- - - - - -

[2] Bateman Manuscript Project, A. Erdélyi ed., Higher Transcendental Functions, (McGraw Hill, New York, 1953). Sections and formulas in this work will be referenced directly by the prefix B.

R_Y only through the Wigner coefficients or 3j-symbols[3,4,5]. The writer's personal preference is for the functions Ω, as they do not necessitate the use of square roots; the place of the 3j-symbols is then taken by un-normalized 3j-coefficients which have the advantage of being integers; as shown in the Appendix, they can be arranged on a 5-dimensional generalization of Pascal's triangle.

For some specific cases expansions of the type (5) have been given before; an addition theorem for solid spherical harmonics ($N=L$ or $N=-L-1$) have been given by Rose[6] and for spherical waves by Friedman and Russek[7]; more recently similar results have been re-derived by Seaton[8]. The radial functions in the expansion (5) for the general case could be obtained by combining these results with those of I, i.e. by considering the product

$$V_{NLM} = r^n \cdot r^L \Omega_L^M(\vartheta,\varphi) \quad , \quad n = N - L \quad , \tag{6}$$

but this would involve the summation of multiply infinite series. Instead, the derivation of the functions R for arbitrary values of N will be based, as in I, on the solution of the set of differential equations

$$\nabla_1^2 V_{NLM} = \nabla_2^2 V_{NLM} \quad , \tag{7a}$$

$$\nabla^2 V_{NLM} = (N-L)(N+L+1) V_{N-2,LM} \quad . \tag{7b}$$

- - - - - -

[3] E. P. Wigner, Group Theory and Its Application to the Quantum Mechanics of Atomic Spectra (Academic Press, New York, 1959).

[4] A. R. Edmonds, Angular Momentum in Quantum Mechanics (Princeton University Press, Princeton, 1957).

[5] M. E. Rose, Elementary Theory of Angular Momentum (John Wiley and Sons, Inc., New York, 1961).

[6] M. E. Rose, J. Maths. and Phys. 37, 215 (1958).

[7] B. Friedman and J. Russek, Quarterly Appl. Maths. 12, 13 (1954).

[8] M. E. Seaton, Proc. Phys. Soc. 77, 84 (1961).

These solutions are again expressible in terms of hypergeometric functions, and leading coefficients are determined by comparison with special known cases; it is found that these constants can always be expressed in terms of integrals of products of three harmonics which may be given in their normalized or un-normalized forms. An alternative method of deriving these coefficients could be based on the transformation properties of the spherical harmonics, but neither this approach, nor any other group-theoretical arguments will be employed in this paper. The only use made of the extensive theory of normalized harmonics[3-5] will be of the relation between the integrals over triple products (Gaunt's coefficients)[9,10] and the 3j-symbols, and the results obtained in terms of the functions Ω will be reformulated in terms of the normalized harmonics Y .

The solutions of the equations (7) satisfying the appropriate continuity conditions will be derived in section 2, and the results discussed in section 3. A selected number of recurrence relations are given in section 4, and in section 5 the formulas are given an operational form applicable to arbitrary functions of r . The special case that one of the vectors points in the direction of the polar axis will be considered in a later paper.

2. Mathematical Derivation

To avoid an excessive use of subscripts, formulas in this section will be derived for the range $r_2 > r_1$ only. The dimensionality of (5) requires that the functions R are of the form

$$R(N,\underset{\sim}{\ell},\underset{\sim}{m};r_1,r_2) = r_1^{\ell'} r_2^{N-\ell'} \sum c_{Ns}(r_1/r_2)^s \quad . \tag{8}$$

The differential equation (7a) substituted in (5) leads to

- - - - - -

[9] J. A. Gaunt, Phil. Trans. Roy. Soc. A 228, 151 (1929).

[10] M. Rotenberg, R. Bivins, N. Metropolis and J. K. Wooten, The 3-j and 6-j symbols, Technology Press, MIT, Cambridge, Mass. (1959).

$$\frac{\partial^2 R}{\partial r_1^2} + \frac{2}{r_1}\frac{\partial^2 R}{\partial r_1} - \ell_1(\ell_1+1)\frac{R}{r_1^2} = \frac{\partial^2 R}{\partial r_2^2} + \frac{2}{r_2}\frac{\partial R}{\partial r_2} - \ell_2(\ell_2+1)\frac{R}{r_2^2} \quad , \tag{9}$$

which together with (8) yields the recurrence relations

$$(s+2)(2\ell_1+s+3)c_{N,s+2} = (N-\ell_1-\ell_2-s)(N-\ell_1+\ell_2+1-s)c_{Ns} \quad . \tag{10}$$

The leading term in the power series (8) is of degree $s = 0$ since the other possible solution, beginning with $s = -2\ell-1$ would lead to a singularity as $r_1 \to 0$. As in I, the solution is best expressed in terms of Gauss' hypergeometric function

$$F(\alpha,\beta;\gamma;z) = \sum_0^\infty (\alpha)_w(\beta)_w\, z^w/\left[(\gamma)_w\, w!\right] \tag{11}$$

where[11]

$$(\alpha)_o = 1 \;;\; (\alpha)_w = (\alpha;w) = \alpha(\alpha+1)\cdots(\alpha+w-1) = \Gamma(\alpha+w)/\Gamma(\alpha) . \tag{12}$$

If we abbreviate

$$\Lambda = \tfrac{1}{2}(L+\ell_1+\ell_2) \;,\; \lambda = \Lambda - L \;,\; \lambda_1 = \Lambda - \ell_1 \;,\; \lambda_2 = \Lambda - \ell_2 \tag{13}$$

and use n as defined in (6), the solution (8) and (10) can be expressed in the form

$$R(N,\underset{\sim}{\ell},\underset{\sim}{m};r_1,r_2) =$$

$$= K(N,\underset{\sim}{\ell},\underset{\sim}{m})\, r_1^{\ell_1}\, r_2^{N-\ell_1}\, F\left[\tfrac{1}{2}(\ell_1+\ell_2-N), \tfrac{1}{2}(\ell_1-\ell_2-1-N); \ell_1+\tfrac{3}{2}; r_1^2/r_2^2\right] \tag{14a}$$

$$= K(N,\underset{\sim}{\ell},\underset{\sim}{m})\, r_1^{\ell_1}\, r_2^{n+L-\ell_1}\, F(\lambda-\tfrac{1}{2}n, -\tfrac{1}{2}-\tfrac{1}{2}n-\lambda_1; \ell_1+\tfrac{3}{2}; r_1^2/r_2^2) \quad . \tag{14b}$$

- - - - - -

[11] The archaic form $(\alpha\,;w)$ will be employed mainly when w carries a subscript.

As the functions Ω_ℓ^m have the parity of ℓ on inversion, $(\vartheta,\varphi) \to (\pi-\vartheta,\pi+\varphi)$, $K(n,\underset{\sim}{\ell},\underset{\sim}{m})$ can take non-zero values only if

$$L - \ell_1 - \ell_2 = \text{even} \quad , \tag{15}$$

and hence all the quantities defined in (13) are integers. The leading coefficients K in (14 a, b) satisfy the recurrence relation, in view of (7b):

$$n(n+1+2L)K(N-2,\underset{\sim}{\ell},\underset{\sim}{m}) = (n-2\lambda)(n+1+2\lambda_1)K(N,\underset{\sim}{\ell},\underset{\sim}{m}) \quad . \tag{16}$$

This means that K depends on n through the factors

$$(-\tfrac{1}{2}n;\lambda)(-\tfrac{1}{2}-\tfrac{1}{2}n-L;\lambda_2) \quad ; \tag{17}$$

the only other way K could depend on n would be through an additional, periodic, factor of period 2; but according to the results of I the factor r^n in (6) does not show any such periodicity and the solid harmonics are independent of n ; hence (17) describes the full dependence of K on n . To find the absolute value of $K(N,\underset{\sim}{\ell},\underset{\sim}{m})$ we first consider the case N = L or n = 0. Making use of (B 3.7.25) and its converse

$$P_\ell^m(\cos\vartheta)e^{im\varphi} = \frac{i^m(\ell+m)!}{2\pi\,\ell!}\int_0^{2\pi}\left[\cos\vartheta + i\sin\vartheta\cos(\varphi-\psi)\right]^\ell e^{im\psi}d\psi \quad , \tag{18a}$$

$$\left[\cos\vartheta + i\sin\vartheta\cos(\varphi-\psi)\right]^\ell = \sum_m \frac{\ell!}{i^m(\ell+m)!}P_\ell^m(\cos\vartheta)e^{im(\varphi-\psi)} \quad , \tag{18b}$$

we obtain for the solid harmonics by means of the binomial theorem

$$\begin{aligned} r^L\Omega_L^M(\vartheta,\varphi) &= \frac{i^M(L+M)!}{2\pi\,L!}\int_0^{2\pi}(z_1+ix_1\cos\psi+iy_1\sin\psi+z_2+ix_2\cos\psi+iy_2\sin\psi)^L e^{iM\psi}d\psi \\ &= \sum (L+M)!\left[(\ell_1+m_1)!(\ell_2+m_2)!\right]^{-1} r_1^{\ell_1} r_2^{\ell_2}\,\Omega_{\ell_1}^{m_1}(\vartheta_1,\varphi_1)\,\Omega_{\ell_2}^{m_2}(\vartheta_2,\varphi_2) \quad , \end{aligned} \tag{19}$$

the sum to be taken over all

$$m_1 + m_2 = M \; ; \; \ell_1 + \ell_2 = L \quad . \tag{20a,b}$$

This is the un-normalized form of Rose's addition theorem[6]. Multiplication by r^n gives rise to terms for which (20b) is no longer satisfied. For positive even n equation (19) of I shows that in the expansion (1) for $|r_1 + r_2|^n$ the radial coefficient of P_λ is $\lambda!(r_1r_2)^\lambda/(\frac{1}{2})_\lambda$ for $\lambda = \frac{1}{2}n$ and vanishes for $\lambda > \frac{1}{2}n$. Hence the leading term in $R(\ell_1+\ell_2,\underset{\sim}{\ell},\underset{\sim}{m})$, in view of (6), (13) and (19) is made up of terms

$$\frac{\lambda! r_1^{\ell_1} r_2^{\ell_2}}{(\frac{1}{2})_\lambda} \sum_\mu (-)^\mu \frac{(L+M)!}{(\lambda_2+m_1+\mu)!(\lambda_1+m_2-\mu)!} \Omega_{\lambda_2}^{m_1+\mu}(1) \; \Omega_{\lambda_1}^{m_2-\mu}(2) \; \Omega_\lambda^{-\mu}(1) \; \Omega_\lambda^{\mu}(2) \quad . \tag{21}$$

The product of two surface harmonics of the same coordinates (ϑ,φ) can be expressed as a sum of spherical harmonics[3-5,9,12,13]

$$\Omega_\ell^m \Omega_\lambda^\mu = \frac{(2\ell)!(2\lambda)!(\ell+\lambda)!(\ell+\lambda-m-\mu)!}{(2\ell+2\lambda)!\,\ell!\,\lambda!(\ell-m)!(\lambda-\mu)!} \Omega_{\ell+\lambda}^{m+\mu} + \cdots \Omega_{\ell+\lambda-2}^{m+\mu} + \cdots \tag{22}$$

This leading term can be found most easily by a comparison of the leading coefficients of $P_\ell^m(x)$, which in view of (2) and Rodrigues' formula (B 3.6.16) are

$$P_\ell^m(x) = (-)^m(1-x^2)^{m/2} \frac{(2\ell)!}{2^\ell \ell!(\ell-m)!} x^{\ell-m} + \cdots \tag{23}$$

The leading coefficient K in (14) for $N = \ell_1 + \ell_2$ thus becomes in view of (21) and (22)

- - - - - -

[12] L. Infeld and T. E. Hull, Rev. Mod. Phys. 23, 21 (1951).

[13] E. A. Hylleraas, Math. Scand. 10, 189 (1962).

$$K(\ell_1+\ell_2,\underset{\sim}{\ell},\underset{\sim}{m}) = (-)^{\Lambda+M} \frac{(L+M)!(\ell_1-m_1)!(\ell_2-m_2)!(2\lambda)!\ell_1!\ell_2!}{\lambda_1!\lambda_2!\lambda!(\frac{1}{2})_\lambda(2\ell_1)!(2\ell_2)!} U\begin{pmatrix} L & \ell_1 & \ell_2 \\ -M & m_1 & m_2 \end{pmatrix} \tag{24}$$

where the symbols U represent the sums

$$U\begin{pmatrix} L & \ell_1 & \ell_2 \\ -M & m_1 & m_2 \end{pmatrix} = \sum_\mu (-)^{-\Lambda+\mu+M} \binom{2\lambda}{\lambda+\mu} \binom{2\lambda_1}{\lambda_1-m_2+\mu} \binom{2\lambda_2}{\lambda_2+m_1+\mu} \tag{25}$$

provided (20a) holds. They are related to the Wigner 3j-symbols[3-5]

$$U\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \left[(2\Lambda+1)! \prod_{s=1}^{3} \frac{(2\lambda_s)!}{(j_s-m_s)!(j_s+m_s)!} \right]^{\frac{1}{2}} \tag{26}$$

where, for this equation only, we have put

$$\Lambda = \tfrac{1}{2}(j_1+j_2+j_3) \quad ; \quad \lambda_s = \Lambda - j_s \geq 0 \ (s=1,2,3) \quad . \tag{27}$$

In the present context these un-normalized 3j-symbols are required for integral values of $\underset{\sim}{\ell}$, $\underset{\sim}{m}$ and $\underset{\sim}{\lambda}$ only, but, as shown in the Appendix, their definition (25) also covers the case of half-integer parameters. For integer Λ they are invariant under a permutation of (1,2,3) in (26) and under a simultaneous change of sign of all the m_s .

The expression (24) can be simplified by the explicit use of Gaunt's coefficients[9,10] for the integral over the product of three associated Legendre functions. If we put

$$I_\Omega\begin{pmatrix} L & \ell & \ell' \\ M & -m & -m' \end{pmatrix} = \int_{-1}^{1} P_L^M(x) P_\ell^{-m}(x) P_{\ell'}^{-m'}(x)\,dx \tag{28}$$

where the azimuthal numbers add up to zero, these integrals can be expressed in terms of the U's as[9]

$$I_\Omega\begin{pmatrix} L & \ell_1 & \ell_2 \\ M & -m_1 & -m_2 \end{pmatrix} = \frac{(-)^{\Lambda}\, 2(\ell_1-m_1)!\,(\ell_2-m_2)!\,(L+M)!\,\Lambda!}{(2\Lambda+1)!\,\lambda_1!\,\lambda_2!\,\lambda!}\, U\begin{pmatrix} L & \ell_1 & \ell_2 \\ M & -m_1 & -m_2 \end{pmatrix}, \tag{29}$$

so that (24) becomes

$$K(\ell_1+\ell_2,\underset{\sim}{\ell},\underset{\sim}{m}) = \frac{(-)^M\,\lambda!\,(\tfrac12;\Lambda+1)}{(\tfrac12;\ell_1)(\tfrac12;\ell_2)}\, I_\Omega\begin{pmatrix} L & \ell_1 & \ell_2 \\ M & -m_1 & -m_2 \end{pmatrix} . \tag{30}$$

Using (17) we find for the leading coefficient for arbitrary N

$$K(N,\underset{\sim}{\ell},\underset{\sim}{m}) = (-)^{\lambda}\,\frac{(-\tfrac12 n;\lambda)(-\tfrac12-\tfrac12 n-L;\lambda_2)}{\lambda!\,(-\tfrac12-\Lambda;\lambda_2)}\,K(\ell_1+\ell_2,\underset{\sim}{\ell},\underset{\sim}{m})$$

$$= (-)^{\lambda+M}\,\frac{(\ell_2+\tfrac12)(-\tfrac12 n;\lambda)(\tfrac32+\tfrac12 n;L)}{(\tfrac12;\ell_1)(\tfrac32+\tfrac12 n;\lambda_1)}\, I_\Omega\begin{pmatrix} L & \ell_1 & \ell_2 \\ M & -m_1 & -m_2 \end{pmatrix}. \tag{31}$$

3. Discussion of the Radial Functions R

According to (14) and (31) the radial functions R in the expansion (5) are given, for $r_2 > r_1$, by

$$R(N,\underset{\sim}{\ell},\underset{\sim}{m};r_1,r_2) = K'(\underset{\sim}{\ell},\underset{\sim}{m})\,R'(N,\underset{\sim}{\ell};r_1,r_2) \tag{32}$$

where

$$K'(\underset{\sim}{\ell},\underset{\sim}{m}) = (-)^{\lambda+M}(\ell_1+\tfrac12)(\ell_2+\tfrac12)\, I_\Omega\begin{pmatrix} L & \ell_1 & \ell_2 \\ M & -m_1 & -m_2 \end{pmatrix} , \tag{33}$$

$$R'(N,\underset{\sim}{\ell};r_1,r_2) = \frac{(-\tfrac12 n;\lambda)(\tfrac32+\tfrac12 n;L)}{(\tfrac12;\ell_1+1)(\tfrac32+\tfrac12 n;\lambda_1)}\, r_1^{\ell_1}\, r_2^{N-\ell_1} \times$$

$$\times F(\lambda-\tfrac12 n,-\tfrac12-\tfrac12 n-\lambda_1;\ell_1+\tfrac32;r_1^2/r_2^2) , \tag{34}$$

and the symbols are explained in (6),(11)-(13), (25),(28) and (29); for $r_1 > r_2$ the subscripts 1 and 2 should be interchanged. The equation

(32) factorizes the functions $R(\underset{\sim}{N},\underset{\sim}{\ell},\underset{\sim}{m})$ into a constant K' independent of N or n and a function R' independent of the azimuthal quantum numbers $\underset{\sim}{m}$. The precise separation is, to some extent, arbitrary as any dependence on $\underset{\sim}{\ell}$ or $\underset{\sim}{\lambda}$ only can be drawn into either factor; the selection (33), (34) was chosen primarily to give the recurrence relations of Section 4 their simplest form. In the case of spherical symmetry

$$L = M = \lambda_1 = \lambda_2 = 0 \quad , \quad m_1 = -m_2 = m \quad ; \quad \ell_1 = \ell_2 = \lambda = \ell$$

$$K' = (-)^{\ell+m}(\ell+\tfrac{1}{2}) \tag{35}$$

and the R' differ from the functions $R_{n\ell}$ of (1) and I only by a factor $(\ell+\frac{1}{2})^{-1}$.

If the spherical harmonics in (5) are given in their normalized form Y_ℓ^m (3c), the analogous radial functions R_Y can be factorized as in (32)

$$R_Y(N,\underset{\sim}{\ell},\underset{\sim}{m};r_1,r_2) = K'_Y(\underset{\wedge}{\ell},\underset{\sim}{m})R'(N,\underset{\sim}{\ell};r_1,r_2) \tag{36}$$

where R' remains unaltered as in (34) whereas in view of (3c) and (26)

$$K'_Y(\underset{\sim}{\ell},\underset{\sim}{m}) = 2\pi(-)^\lambda \ (LM|Y_{\ell_1}^{m_1}|\ell_2 m_2) \quad . \tag{37}$$

Here

$$(LM|Y_\ell^m|\ell' m') = (-)^M\left[(2\ell+1)(2\ell'+1)(2L+1)/4\pi\right]^{\frac{1}{2}}\begin{pmatrix} L & \ell & \ell' \\ -M & m & m'\end{pmatrix}\begin{pmatrix} L & \ell & \ell' \\ 0 & 0 & 0\end{pmatrix}$$

$$= \iint\left[Y_L^M(\vartheta,\varphi)\right]^* Y_\ell^m(\vartheta,\varphi)Y_{\ell'}^{m'}(\vartheta,\varphi)\sin\vartheta\, d\vartheta\, d\varphi \tag{38}$$

is the integral of the product of three normalized harmonics taken over the whole unit sphere[10]. In view of the properties of the 3j-symbols the coefficients K', and hence the radial functions R, will be non-zero only if the conditions

$$|\ell_1-\ell_2| \le L \le \ell_1+\ell_2 \tag{39}$$

are satisfied as well as (15) and (20a). The functions R will also vanish, in view of (13), (32) and (34), if

$$L \le N < \ell_1+\ell_2 \quad , \quad n \ \text{even} \tag{40a}$$

or

$$-L \le N+1 < \ell_1-\ell_2 \quad , \quad n \ \text{odd} \quad , \quad r_2 > r_1 \quad . \tag{40b}$$

The hypergeometric series are polynomials if

$$N \ge \ell_1+\ell_2 \quad , \quad n \ \text{even} \quad \text{or} \quad N \ge \ell_1-\ell_2-1 \quad , \quad n \ \text{odd} \quad ; \tag{41}$$

if either equality holds, they reduce to the leading term unity. The particular case $N = L$ has been discussed in (19) and (20); if $N = -L-1$, the only non-vanishing functions in (5) for $r_2 > r_1$ are those for which $\ell_2 = L + \ell_1$, and for these we have, in view of (22) or from [9,11]

$$I_{\Omega}\begin{pmatrix} L, \ell_1, L+\ell_1 \\ M, -m_1, m_1-M \end{pmatrix} = (-)^{M-m_1} \frac{2(2L)!(2\ell_1)!(\ell_1+L)!(\ell_1+L+m_1-M)!}{(2\ell_1+2L+1)!L!\ell_1!(L-M)!(\ell_1+m_1)!} \tag{42}$$

so that (5) and (32)-(34) yield

$$r^{-L-1}\Omega_L^M(\vartheta,\varphi) = \sum_{\ell,m} (-)^{\ell+m} \frac{(\ell+L+m-M)!}{(\ell+m)!(L-M)!} r_1^{\ell} r_2^{-L-\ell-1} \Omega_\ell^m(\vartheta_1,\varphi_1)\Omega_{L+\ell}^{M-m}(\vartheta_2,\varphi_2) \quad . \tag{43}$$

This corresponds to the expansion given by Rose for normalized "irregular" solid harmonics[6].

As in I the transformation theory of the hypergeometric functions can be applied to the expression (34) for the functions R'. Thus (B 2.9.1,2) or eq. (20a) of I, leads to

$$R'(N,\underset{\sim}{\ell};r_1,r_2) = \frac{(-\tfrac{1}{2}n;\lambda)(\tfrac{3}{2}+\tfrac{1}{2}n;L)}{(\tfrac{1}{2};\ell_1+1)(\tfrac{3}{2}+\tfrac{1}{2}n;\lambda_1)} \frac{r_1^{\ell_1}(r_2^2-r_1^2)^{N+2}}{r_2^{N+4+\ell_1}} \times$$
$$\times F(\Lambda+2+\tfrac{1}{2}n,\tfrac{3}{2}+\tfrac{1}{2}n+\lambda_2;\ell_1+\tfrac{3}{2};r_1^2/r_2^2) \tag{44}$$

which shows that the radial functions are also rational in r_1 and r_2 if $\tfrac{1}{2}(\ell_1+\ell_2+N)+1$ or $\tfrac{1}{2}(\ell_1-\ell_2+N+1)$ are negative integers. Similarly (B 2.10.1) or (20b) of I yield

$$R'(N,\underset{\sim}{\ell};r_1,r_2) = \frac{2^{n+1}(-\tfrac{1}{2}n;\lambda)(\tfrac{3}{2}+\tfrac{1}{2}n;L)(2+n;L)}{(1+\tfrac{1}{2}n;\Lambda+1)(\tfrac{3}{2}+\tfrac{1}{2}n;\lambda_1)(\tfrac{3}{2}+\tfrac{1}{2}n;\lambda_2)} r_1^{\ell_1} r_2^{N-\ell_1} \times$$
$$\times F(\lambda-\tfrac{1}{2}n,-\tfrac{1}{2}-\tfrac{1}{2}n-\lambda_1;-n-1-L;(r_2^2-r_1^2)/r_2^2) +$$
$$- \frac{(-)^{\lambda_2}(\tfrac{3}{2}+\tfrac{1}{2}n;L)}{(n+2;L+1)2^{n+2}} \frac{r_1^{\ell_1}(r_2^2-r_1^2)^{N+2}}{r_2^{N+4+\ell_1}} \times$$
$$\times F(\Lambda+2+\tfrac{1}{2}n,\tfrac{3}{2}+\tfrac{1}{2}n+\lambda_2;n+3+L;\frac{r_2^2-r_1^2}{r_2^2}) \tag{45}$$

where the coefficients have been simplified in view of the properties of the gamma function, (B 1.2.6) and (B 1.3.15) or (23) and (25) of I. This equation shows the nature of the branch point as r_1 approaches r_2; the difficulties arising for integer values of n have been discussed in I, following eq. (22); the result is either a polynomial or a series involving logarithmic terms. In the case $L = 0$, it was shown in I that by means of quadratic transformations applied to the hypergeometric functions the radial functions $R_{n\ell}$ could be expressed in several forms symmetric in r_1 and r_2, involving power series in $r_1r_2/(r_1+r_2)^2$ or in $r_1r_2/(r_1^2+r_2^2)$. The same transformations can be applied whenever $\ell_1 = \ell_2$, regardless of the value of L; for general values of ℓ_1 and ℓ_2 (34) shows that even the leading coefficients are different as $r_1 < r_2$ or $r_1 > r_2$. In consequence it is unlikely that analogous simple symmetric expansions exist in the general case. On the other hand the leading coefficients in (45) are invariant for $r_1 \gtrless r_2$, and together with the symmetry of the recurrence relations derived below, this suggests the existence of symmetric expansions involving power series in the two arguments $r_1 r_2/(r_1^2+r_2^2)$ and $(r_1^2-r_2^2)/(r_1^2+r_2^2)$ or similar variables, though presumably involving the one variable only to a finite power depending on $|\ell_1-\ell_2|$. So far the writer has been unable to derive such expansions.

Quadratic transformations for arbitrary hypergeometric functions have recently been derived by Kuipers and Meulenbeld[14] in terms of generalized hypergeometric functions or MacRobert's E-functions, (cf. (B 4) and (B 5)). This generalization, however, is not quite relevant to the problem at this stage, as it corresponds to a generalization of the transformation from (27a) to (27b) of I, and not of the transformation from (19) to (27).

It might be considered that the expansion (5) would simplify if one of the vectors, say r_1, points in the direction of the polar axis; for this choice all the Legendre functions of $\cos\vartheta_1$ are 1 or 0, according as $m_1 = 0$ or $m_1 \neq 0$, and hence for all non-vanishing terms $m_2 = M$. The individual terms in (5) are therefore considerably simpler than in the general case; on the other hand, because of the restrictions imposed on r_1 the rotational quantum number ℓ_1 ceases to be meaningful and any consistent expansion making use of this restriction should reasonable involve an implicit summation over ℓ_1, i.e. over products involving 3j-symbols. From an analytic point of view these symbols are generalized hypergeometric series (cf. (B 4) and [9,15]) of unit argument and all integer parameters, and any expansion involving such functions is likely to lead back to functions of at least the same, and possibly higher, complexity. This has indeed been found to be the case, and in order not to complicate any further the mathematical

------

[14] L. Kuipers and B. Meulenbeld, J. London Math. Soc. 35, 221 (1960).

[15] P. E. Bryant, Tables of Wigner 3j-symbols, University of Southampton, Research Report 60-1 (1960).

apparatus required for the present paper, the case $\vartheta_1 = 0$ will be considered separately in a later publication.

4. Recurrence Relations

The relations between contiguous hypergeometric functions (B 2.8.28-45) can be used, as in I, to derive linear recurrence relations between any three radial functions R' for which L, ℓ_1, ℓ_2 and $\frac{1}{2}N$ differ by integers only; the recurrence formulas between the coefficients K' of (33) or (37) are known from the theory of angular momentum[3-5,9,10]. Equation (14a) shows that the functions F depend on n and L only through their sum N; according to (34)

$$\frac{R'(N,L+2,\ell_1,\ell_2)}{R'(N,L,\ell_1,\ell_2)} = \frac{3+N+L}{L-N} = -\frac{3+n+2L}{n} \quad . \tag{46}$$

It is therefore sufficient to drive any further relations for changing values of the angular quantum numbers L, ℓ_1 and ℓ_2 only, leaving

$$n = N-L = \text{const} \quad ; \tag{47}$$

the value of N can then be increased or decreased in steps of 2 by means of (46). In view of the larger number of independent parameters, the number of recurrence relations for even small changes in $\underset{\sim}{\ell}$ will be considerable; we therefore confine our attention to the following special cases:

(i) Between any two of the three functions R', none of the numbers L, ℓ_1 and ℓ_2 differ by more than unity.

(ii) One of the angular quantum numbers remains constant, the second varies by at most unity, and the third by at most two units.

There are 8 inequivalent 3-term recurrence relations of type (i) and 12 of type (ii); for the sake of brevity only those parameters will be indicated which differ from L, ℓ_1, ℓ_2, e.g. $R'(L+,\ell_1-) = R'(L+1,\ell_1-1,\ell_2)$ (cf. B 2.9), and N is understood to vary according to (47). The formulas are:

$$(\tfrac{3}{2}+\tfrac{1}{2}n+L)(r_2{}^2-r_1{}^2)R' =$$

$$= (\lambda_1+\tfrac{3}{2}+\tfrac{1}{2}n)r_2R'(L+,\ell_2+) - (\lambda_2+\tfrac{3}{2}+\tfrac{1}{2}n)r_1R'(L+,\ell_1+) \tag{48a}$$

$$= (\lambda-1-\tfrac{1}{2}n)r_2R'(L+,\ell_2-) - (\Lambda+2+\tfrac{1}{2}n)r_1R'(L+,\ell_1+) \tag{48b}$$

$$= (\Lambda+2+\tfrac{1}{2}n)r_2R'(L+,\ell_2+) - (\lambda-1-\tfrac{1}{2}n)r_1R'(L+,\ell_1-) \tag{48c}$$

$$= -(\tfrac{3}{2}+\lambda_2+\tfrac{1}{2}n)r_2R'(L+,\ell_2-) + (\lambda_1+\tfrac{3}{2}+\tfrac{1}{2}n)r_1R'(L+,\ell_1-) \quad ; \tag{48d}$$

$$(\tfrac{1}{2}+\tfrac{1}{2}n+L)^{-1}R' =$$

$$= (\lambda-\tfrac{1}{2}n)^{-1}\left[r_2R'(L-,\ell_2+) + r_1R'(L-,\ell_1+)\right] \tag{49a}$$

$$= (\tfrac{1}{2}+\tfrac{1}{2}n+\lambda_1)^{-1}\left[r_2R'(L-,\ell_2-) - r_1R'(L-,\ell_1+)\right] \tag{49b}$$

$$= (\tfrac{1}{2}+\tfrac{1}{2}n+\lambda_2)^{-1}\left[-r_2R'(L-,\ell_2+) + r_1R'(L-,\ell_1-)\right] \tag{49c}$$

$$= (\Lambda+1+\tfrac{1}{2}n)^{-1}\left[r_2R'(L-,\ell_2-) + r_1R'(L-,\ell_1-)\right] \quad ; \tag{49d}$$

$$(\ell_2+\tfrac{1}{2})R' =$$

$$= (\tfrac{1}{2}+\tfrac{1}{2}n+L)r_2\left[R'(L-,\ell_2+) + R'(L-,\ell_2-)\right] \tag{50a}$$

$$= r_2\left[(\Lambda+2+\tfrac{1}{2}n)(\lambda_1+\tfrac{3}{2}+\tfrac{1}{2}n)R'(L+,\ell_2+) - (\lambda-1-\tfrac{1}{2}n)(\lambda_2+\tfrac{3}{2}+\tfrac{1}{2}n)\times \times R'(L+,\ell_2-)\right] / \left[(\tfrac{3}{2}+\tfrac{1}{2}n+L)(r_2{}^2-r_1{}^2)\right] \tag{50b}$$

$$= (r_2/r_1)\left[-(\lambda_1+\tfrac{3}{2}+\tfrac{1}{2}n)R'(\ell_1-,\ell_2+) + (\lambda-1-\tfrac{1}{2}n)R'(\ell_1-,\ell_2-)\right] \tag{51a}$$

$$= (r_2/r_1)\left[(\Lambda+2+\tfrac{1}{2}n)R'(\ell_1+,\ell_2+) + (\tfrac{3}{2}+\tfrac{1}{2}n+\lambda_2)R'(\ell_1+,\ell_2-)\right] \quad ; \tag{51b}$$

$(L+n+2)(\frac{3}{2}+\frac{1}{2}n+L)\,r_2R' =$

$$= (\tfrac{1}{2}+\tfrac{1}{2}n+L)_2(r_2{}^2-r_1{}^2)R'(L-,\ell_2-) + (\lambda-1-\tfrac{1}{2}n)(\lambda_2+\tfrac{1}{2}n+\tfrac{3}{2})R'(L+,\ell_2-) \qquad (52a)$$

$$= -(\tfrac{1}{2}+\tfrac{1}{2}n+L)_2(r_2{}^2-r_1{}^2)R'(L-,\ell_2+) + (2+\Lambda+\tfrac{1}{2}n)(\lambda_1+\tfrac{1}{2}n+\tfrac{3}{2})R'(L+,\ell_2+)\ . \qquad (52b)$$

The other 6 relations of the type (ii) are obtained by an interchange of the subscripts 1 and 2 in (50)-(52). Although the resulting equations are invariant on interchanging (ℓ_1, r_1) and (ℓ_2, r_2), their derivation is not symmetrical; thus (50) follows from (B 2.8.32,37), but the corresponding equations for varying ℓ_1 from

$$\gamma(\gamma-1)\left[F(\gamma-) - F\right] = \alpha\beta zF(\alpha+,\beta+,\gamma+) \qquad (53)$$

and from (B 2.9.1,2). The equations (48a,b) follow from (B 2.8.38,43), and (49c,d) from (B 2.8.35,42); the remaining relations are derived from these by linear elimination, though to prove (51) the values of L in (48) and (49) must be lowered or raised.

It should be remembered in applying the recurrence relations (48)-(52) that they do not apply to the full radial functions R of (32); these latter will vanish whenever the triangular condition (39) is violated because of the factor K' in (33), whereas the factors R' will have perfectly well defined, usually non-zero, values in accordance with (46) regardless of the relative values of L, ℓ_1, and ℓ_2 provided only (15) is satisfied.

5. An Operational Expansion for Arbitrary Functions

As in I the way in which the power N enters into the expressions (32)-(34) allows the functions $R'(N,\underset{\sim}{\ell};r_1,r_2)$ to be expressed in operational form. For $r_2 > r_1$ the expressions differ according to the relative magnitudes of L and ℓ_2. For the factor in the general term in (34), which depends on N, we have using (11)-(14)

$$(-)^{\ell_1}\, 2^{\ell_1+2s} (\tfrac{1}{2}L-\tfrac{1}{2}N;\lambda+s)(-\tfrac{1}{2}-\tfrac{1}{2}N-\tfrac{1}{2}L;\lambda_2+s)\, r_2^{N-\ell_1-2s} =$$

$$= r_2^{-1-\ell_2}\left(\frac{1}{r_2}\frac{\partial}{\partial r_2}\right)^{L-\ell_2} r_2^{L}\left[\frac{\partial^2}{\partial r_2^{\,2}} - \frac{L(L+1)}{r_2^{\,2}}\right]^{\lambda+s} r^{N+1}\ , \quad L \geq \ell_2 \qquad (54a)$$

$$= r_2\left(\frac{1}{r_2}\frac{\partial}{\partial r_2}\right)^{\ell_2-L} r_2^{-1-L}\left[\frac{\partial^2}{\partial r_2^{\,2}} - \frac{L(L+1)}{r_2^{\,2}}\right]^{\lambda_2+s} r^{N+1}\ , \quad L \leq \ell_2\ . \qquad (54b)$$

Hence any function $f(r)$ which can be represented as a power series in r we can expand, in analogy to (5),

$$f(r)\,\Omega_L^{M}(\vartheta,\varphi) = \sum K'(\underset{\sim}{\ell},\underset{\sim}{m})\, f'(\underset{\sim}{\ell};r_1,r_2)\ \Omega_{\ell_1}^{m_1}(\vartheta_1,\varphi_1)\ \Omega_{\ell_2}^{m_2}(\vartheta_2,\varphi_2) \qquad (55)$$

where K' is given by (33), or by (37) if normalized surface harmonics are used. For the radial functions we obtain from (34) and (54)

$$f'(\underset{\sim}{\ell};r_1,r_2) = 2(-)^{\lambda}\sum_s \frac{r_1^{\ell_1+2s}\, g_s(\underset{\sim}{\ell};r_2)}{(2\ell_1+2s+1)!!\,(2s)!!} \qquad r_2 > r_1 \qquad (56)$$

(for the double factorials see (43) of I) where

$$g_s(\underset{\sim}{\ell},r_2) = r_2^{-1-\ell_2}\left(\frac{1}{r_2}\frac{d}{dr_2}\right)^{L-\ell_2} r_2^{L}\left[\frac{d^2}{dr_2^{\,2}} - \frac{L(L+1)}{r_2^{\,2}}\right]^{\lambda+s}\left[r_2 f(r_2)\right]\ , \quad L \geq \ell_2 \qquad (57a)$$

$$= r_2^{\ell_2}\left(\frac{1}{r_2}\frac{d}{dr_2}\right)^{\ell_2-L} r_2^{-1-L}\left[\frac{d^2}{dr_2^{\,2}} - \frac{L(L+1)}{r_2^{\,2}}\right]^{\lambda_2+s}\left[r_2 f(r_2)\right]\ , \quad L \leq \ell_2\ . \qquad (57b)$$

Alternatively the powers of the operator $(r_2^{-1}d/dr_2)$ can be put last with the result

$$g_s(\underset{\sim}{\ell},r_2) = \frac{1}{r_2}\left[\frac{d^2}{dr_2^{\,2}} - \frac{\ell_2(\ell_2+1)}{r_2^{\,2}}\right]^{\lambda+s} \frac{1}{r_2^{\ell_2}}\left[\frac{1}{r_2}\frac{d}{dr_2}\right]^{L-\ell_2}\left[r_2^{L+1} f(r_2)\right]\ , \quad L \geq \ell_2 \qquad (58a)$$

$$= \frac{1}{r_2}\left[\frac{d^2}{dr_2^{\,2}} - \frac{\ell_2(\ell_2+1)}{r_2^{\,2}}\right]^{\lambda_2+s} r_2^{\ell_2+1}\left[\frac{1}{r_2}\frac{d}{dr_2}\right]^{\ell_2-L}\left[\frac{f(r_2)}{r_2^{L}}\right]\ , \quad L \leq \ell_2\ . \qquad (58b)$$

The quadratic operators occurring in (57) and (58) can be factorized, but not expressed as squares; hence the operational factorization of f_ℓ in (48) of I in terms of Bessel functions of a differential operator does not appear to have a simple analogue in the general case.

The expressions (56)-(58) factorize analytically if f is a spherical Bessel function

$$f(r) = w_L(kr) \quad , \quad w_L = i_L, y_L, h_L^{(1)}, h_L^{(2)} \tag{59}$$

in the usual notation, satisfying

$$\left[d^2/dr^2 - L(L+1)/r^2\right]\left[rf(r)\right] = -k^2 rf(r) \ . \tag{60}$$

In view of (B 7.2.44-46,52,53) and (B 7.11.5-13) we have

$$\begin{aligned} (z^{-1}d/dz)^s\left[z^{-\ell}w_\ell(z)\right] &= (-)^s z^{-\ell-s}w_{\ell+s}(z) \quad , \\ (z^{-1}d/dz)^s\left[z^{1+\ell}w_\ell(z)\right] &= z^{1+\ell-s}w_{\ell-s}(z) \quad , \end{aligned} \tag{61}$$

so that (56) and (57) or (58) yield

$$f'(\underset{\sim}{\ell};r_1,r_2) = 2\,j_{\ell_1}(kr_1)w_{\ell_2}(kr_2) \quad , \quad r_2 \geq r_1 \ . \tag{62}$$

Substituting this into (55) and making use of (33) or (37) we find an expansion equivalent to the expansion theorem for spherical waves derived by Friedman and Russek[7]; apparent discrepancies are due to the differing definitions of the spherical harmonics. For modified spherical Bessel functions the expressions corresponding to (62) become in view of (B 2.7.19-22)

$$\begin{aligned} f &= i_\ell(kr) \quad ; \quad f' = 2(-)^{\lambda}\, i_{\ell_1}(kr_1)i_{\ell_2}(kr_2) \quad , \\ f &= k_\ell(kr) \quad ; \quad f' = 2(-)^{\lambda_2} i_{\ell_1}(kr_1)k_{\ell_2}(kr_2) \quad , \quad r_2 \geq r_1 \ . \end{aligned} \tag{63}$$

It should be borne in mind that the actual signs in the expansion (55) are not necessarily those given in (62) or (63) in view of the changes in sign occurring in (33) and (37).

The algebraic recurrence relations (48)-(52) are not directly applicable to the operational expansion terms (55)-(58); it should, nevertheless, be possible to derive recurrence relations for the functions $f'(\underset{\sim}{\ell})$, if necessary involving more than three terms. Such relations might lead to a considerable simplification in the evaluation of the radial functions.

Appendix: The Un-Normalized 3j-symbols

The theory of the Wigner 3j-symbols is well established[3-5] and their values have been extensively tabulated[10,15]; it may therefore appear futile to return to the use of un-normalized harmonics and 3j-symbols associated with these. However the use of integers has its advantages, compared with expressions involving square roots; and from this point of view the symbols U introduced in (25) may be found useful. Their definition is easily generalized to any set of integral or half-integral parameters (j_s, m_s), provided $m_1 + m_2 + m_3 = 0$ and all the $(j_s + m_s)$ as well as $2\Lambda = j_1 + j_2 + j_3$ are integers and the triangular relation (39) holds for the j's. Using the abbreviations (27) we define

$$U\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \sum_{\mu} (-)^{\sigma - \Lambda + \mu} \binom{2\lambda_1}{\lambda_1 + \mu} \binom{2\lambda_2}{\lambda_2 - m_3 + \mu} \binom{2\lambda_3}{\lambda_3 + m_2 + \mu} \qquad \text{(A1)}$$

where

$$\sigma \equiv 2j_1 - m_2 + m_3 \equiv m_1 + 2m_3 \equiv -m_1 - 2m_2 \pmod 2 \qquad \text{(A2)}$$

and the sum is to be taken over all integral or half-integral values of μ (depending on λ_1) for which all the binomial coefficients are non-zero. The relation of these quantities to Wigner's normalized 3j-symbols[3-5] is given in (26); like the latter they are invariant under a cyclic permutation of (1, 2, 3) and are multiplied by $(-)^{2\Lambda}$ for a non-cyclic permutation or for the transformation $\underset{\sim}{m} \to -\underset{\sim}{m}$. On the other hand the constant numerator in the sum (A1) destroys the Regge symmetries[16] of the symbols under permutation of the triples $2\lambda_s$, $j_s + m_s$, $j_s - m_s$.

Against this loss of symmetry, the definition (A1) has the advantage that all the terms in the sum are integers which even for $J = 32$ never exceed 10^9. For $j_1 = j_2 + j_3$, i.e. $\lambda_1 = 0$, the sum reduces to a single term

\- - - - - -

[16] T. Regge, Nuovo Cimento 10, 545 (1958).

$$U\begin{pmatrix} j_2+j_3, j_2, j_3 \\ -m_2-m_3, m_2, m_3 \end{pmatrix} = (-)^{j_2+j_3-m_2+m_3} \begin{pmatrix} 2j_2 \\ j_2+m_2 \end{pmatrix}\begin{pmatrix} 2j_3 \\ j_3+m_3 \end{pmatrix} \quad . \tag{A3}$$

In view of the property of the binomial coefficients

$$\begin{pmatrix} N \\ M \end{pmatrix} = \begin{pmatrix} N-1 \\ M-1 \end{pmatrix} + \begin{pmatrix} N-1 \\ M \end{pmatrix} \tag{A4}$$

the definition (A1) entails the recurrence formula

$$U\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = U\begin{pmatrix} j_1, j_2-\frac{1}{2}, j_3-\frac{1}{2} \\ m_1, m_2-\frac{1}{2}, m_3+\frac{1}{2} \end{pmatrix} - U\begin{pmatrix} j_1, j_2-\frac{1}{2}, j_3-\frac{1}{2} \\ m_1, m_2+\frac{1}{2}, m_3-\frac{1}{2} \end{pmatrix} \quad ; \tag{A5}$$

the equivalent formula for the normalized 3j-symbols has been given by Edmonds[4]. Apart from signs, the relation (A5) is similar to that obtaining in Pascal's triangle; and since for $j_3 = 0$ the absolute values of U are binomial coefficients, the whole set of coefficients U can be regarded as a five-dimensional generalization of Pascal's triangle. The numbers can thus be generated by means of (A3) and (A5); for work with electronic computers this would appear more convenient than the more usual representation of the squares of the normalized symbols as products and ratios of powers of primes[10,15]. A more detailed discussion of the symbols U will be given elsewhere.